NUCLEATION OF WATER-SOLUBLE WHISKER CRYSTALS

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1. Introduction. Whisker crystals (whiskers) of water-soluble materials, such as alkali halides, are grown out from a film of the solution by evaporation of water[1]. Essentially, they contain no axial dislocations, which suggests no aids of an axial screw dislocation are needed for the growth[2-6]. The growth process of the whiskers is relatively simple, since the vaporization of the water is the only one chemical reaction relating to the growth. The actual growth process, however, is not so simple. Their growth point can be either their tips[7,8] or roots[5] depending on the growth conditions. Regardless of the growth directions, the growth of whiskers might start from a small crystal of nearly isotropic shape, and then grow into whiskers. In the initial stage, the mechanism of morphological change has not been clarified.

2. Growth Model. A thin layer of saturated solution of the whisker-forming material covers a smooth substrate. Then a microcrystal of simple cubic structure with six {100} dislocation-free surfaces nucleates in the solution. The evaporation of the solvent is accelerated on the top of the microcrystal by increasing the effective supersaturation in the atmosphere due to Gibbs-Thomson's effect, since the vapor-liquid (V-L) interface forms a localized convex region as shown in Fig.1. In a circle of concave region, the supersaturation is decreased.

3. Computation. The sites of the evaporation and the condensation of solvent molecules were chosen at random in the V-L interface with the weight of vaporization probability related with the local curvature. Then a three-dimensional random walk model simulated a diffusion process by which the increase and the decrease in the supersaturation diffused from the interface within the liquid layer. The direction of each walking step was chosen at random in the spherical coordination. The degree of supersaturation in the liquid was set first just below the critical value to form a two-dimensional nucleation on the perfect {100} surfaces.

4. Results and Discussion. The crystal was able to elongate only when the surface diffusion was considered. Fig.2 shows a successive process of the shape change

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with single nucleation layer-by-layer growth conditions, where the starting microcrystal is a small cube with the height $h = 0.1\ W_L$, where W_L is the width of the liquid layer. As shown in the figure, the microcrystal tended to grow unidirectional, without any aid of dislocations. The present process relates to the earliest stage of the whisker growth. After that the microcrystal may grow into a whisker with any possible growth mechanism. As examples, both "root growth with the floating root in the liquid" [5] and "tip growth with a liquid layer" [7] mechanisms for whisker growth can follow the present nucleation process.

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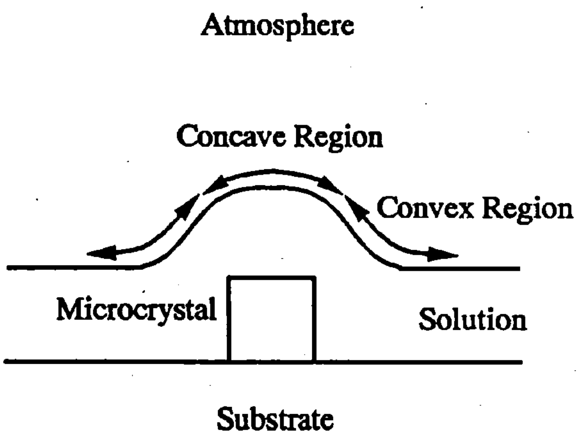

Fig. 1

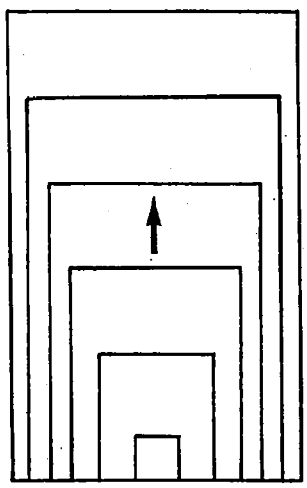

Fig. 2